# Prescription for experimental determination of the dynamics of a quantum black box

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We give an explicit prescription for experimentally determining the evolution operators which completely describe the dynamics of a quantum mechanical black box – an arbitrary open quantum system. We show necessary and sufficient conditions for this to be possible, and illustrate the general theory by considering specifically one and two quantum bit systems. These procedures may be useful in the comparative evaluation of experimental quantum measurement, communication, and computation systems.

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### I. INTRODUCTION

Consider a black box with an input and an output. Given that the transfer function is linear, if the dynamics of the box are described by classical physics, well known recipes exist to completely determine the response function of the system. Now consider a quantum-mechanical black box whose input may be an arbitrary quantum state (in a finite dimensional Hilbert space), with internal dynamics and an output state (of same dimension as the input) determined by quantum physics. The box may even be connected to an external reservoir, or have other inputs and outputs which we wish to ignore. Can we determine the quantum transfer function of the system?

The answer is yes. Simply stated, the most arbitrary transfer function of a quantum black box is to map one density matrix into another,  $\rho_{in} \rightarrow \rho_{out}$ , and this is determined by a linear mapping  $\mathcal{E}$  which we shall give a prescription for obtaining. The interesting observation is that this black box may be an attempt to realize a useful quantum device. For example, it may be a quantum cryptography channel [1,2] (which might include an eavesdropper!), a quantum computer in which decoherence occurs, limiting its performance [3,4], or just an imperfect quantum logic gate [5,6], whose performance you wish to characterize to determine its usefulness.

How many parameters are necessary to describe a quantum black box acting on an input with a state space of N dimensions? And how may these parameters be experimentally determined? Furthermore, how is the resulting description of  $\mathcal{E}$  useful as a performance characterization?

We consider these questions in this paper. After summarizing the relevant mathematical formalism, we prove

that  $\mathcal{E}$  may be determined completely by a matrix of complex numbers  $\chi$ , and provide an accessible experimental prescription for obtaining  $\chi$ . We then give explicit constructions for the cases of one and two quantum bits (qubits), and then conclude by describing related performance estimation quantities derivable from  $\chi$ .

# II. STATE CHANGE THEORY

A general way to describe the state change experienced by a quantum system is by using quantum operations, sometimes also known as superscattering operators or completely positive maps. This formalism is described in detail in [7], and is given a brief but informative review in the appendix to [8]. A quantum operation is a linear map  $\mathcal{E}$  which completely describes the dynamics of a quantum system,

$$\rho \to \frac{\mathcal{E}(\rho)}{\operatorname{tr}(\mathcal{E}(\rho))}$$
 (2.1)

A particularly useful description of quantum operations for theoretical applications is the so-called *operator-sum* representation:

$$\mathcal{E}(\rho) = \sum_{i} A_{i} \rho A_{i}^{\dagger} \,. \tag{2.2}$$

The  $A_i$  are operators acting on the system alone, yet they completely describe the state changes of the system, including any possible unitary operation (quantum logic gate), projection (generalized measurement), or environmental effect (decoherence). In the case of a "nonselective" quantum evolution, such as arises from uncontrolled interactions with an environment (as in the decoherence of quantum computers), the  $A_i$  operators satisfy an additional completeness relation,

$$\sum_{i} A_i^{\dagger} A_i = I. \tag{2.3}$$

This relation ensures that the trace factor  $\operatorname{tr}(\mathcal{E}(\rho))$  is always equal to one, and thus the state change experienced by the system can be written

$$\rho \to \mathcal{E}(\rho)$$
. (2.4)

Such quantum operations are in a one to one correspondence with the set of transformations arising from the joint unitary evolution of the quantum system and an initially uncorrelated environment [7]. In other words, the quantum operations formalism also describes the master equation and quantum Langevin pictures widely used in quantum optics [9,10], where the system's state change arises from an interaction Hamiltonian between the system and its environment [11].

Our goal will be to describe the state change process by determining the operators  $A_i$  which describe  $\mathcal{E}$ , (and until Section VI we shall limit ourselves to those which satisfy Eq.(2.3)). Once these operators have been determined many other quantities of great interest, such as the fidelity, entanglement fidelity and quantum channel capacity can be determined. Typically, the  $A_i$  operators are derived from a theoretical model of the system and its environment; for example, they are closely related to the Lindblad operators. However, what we propose here is different: to determine systematically from experiment what the  $A_i$  operators are for a specific quantum black box.

# III. GENERAL EXPERIMENTAL PROCEDURE

The experimental procedure may be outlined as follows. Suppose the state space of the system has N dimensions; for example, N=2 for a single qubit.  $N^2$  pure quantum states  $|\psi_1\rangle\langle\psi_1|,\ldots,|\psi_{N^2}\rangle\langle\psi_{N^2}|$  are experimentally prepared, and the output state  $\mathcal{E}(|\psi_j\rangle\langle\psi_j|)$  is measured for each input. This may be done, for example, by using quantum state tomography [12–14]. In principle, the quantum operation  $\mathcal{E}$  can now be determined by a linear extension of  $\mathcal{E}$  to all states. We prove this below.

The goal is to determine the unknown operators  $A_i$  in Eq.(2.2). However, experimental results involve numbers (not operators, which are a theoretical concept). To relate the  $A_i$  to measurable parameters, it is convenient to consider an equivalent description of  $\mathcal{E}$  using a fixed set of operators  $\tilde{A}_i$ , which form a basis for the set of operators on the state space, so that

$$A_i = \sum_m a_{im} \tilde{A}_m \tag{3.1}$$

for some set of complex numbers  $a_{im}$ . Eq.(2.2) may thus be rewritten as

$$\mathcal{E}(\rho) = \sum_{mn} \tilde{A}_m \rho \tilde{A}_n^{\dagger} \chi_{mn} , \qquad (3.2)$$

where  $\chi_{mn} \equiv \sum_i a_{im} a_{in}^*$  is a "classical" error correlation matrix which is positive Hermitian by definition. This shows that  $\mathcal{E}$  can be completely described by a complex number matrix,  $\chi$ , once the set of operators  $\tilde{A}_i$  has been fixed. In general,  $\chi$  will contain  $N^4 - N^2$  independent parameters, because a general linear map of N by N matrices to N by N matrices is described by  $N^4$  independent parameters, but there are  $N^2$  additional constraints due to the fact that the trace of  $\rho$  remains one. We will show how to determine  $\chi$  experimentally, and then show how an operator sum representation of the form Eq.(2.2) can be recovered once the  $\chi$  matrix is known.

Let  $\rho_j$ ,  $1 \leq j \leq N^2$  be a set of linearly independent basis elements for the space of  $N \times N$  matrices. A convenient choice is the set of projectors  $|n\rangle\langle m|$ . Experimentally, the output state  $\mathcal{E}(|n\rangle\langle m|)$  may be obtained by preparing the input states  $|n\rangle$ ,  $|m\rangle$ ,  $|n_+\rangle = (|n\rangle +$  $|m\rangle)/\sqrt{2}$ , and  $|n_-\rangle = (|n\rangle + i|m\rangle)/\sqrt{2}$  and forming linear combinations of  $\mathcal{E}(|n\rangle\langle n|)$ ,  $\mathcal{E}(|m\rangle\langle m|)$ ,  $\mathcal{E}(|n_+\rangle\langle n_+|)$ , and  $\mathcal{E}(|n_-\rangle\langle n_-|)$ . Thus, it is possible to determine  $\mathcal{E}(\rho_j)$  by state tomography, for each  $\rho_j$ .

Furthermore, each  $\mathcal{E}(\rho_j)$  may be expressed as a linear combination of the basis states,

$$\mathcal{E}(\rho_j) = \sum_k \lambda_{jk} \rho_k \,, \tag{3.3}$$

and since  $\mathcal{E}(\rho_j)$  is known,  $\lambda_{jk}$  can thus be determined. To proceed, we may write

$$\tilde{A}_m \rho_j \tilde{A}_n^{\dagger} = \sum_k \beta_{jk}^{mn} \rho_k \,, \tag{3.4}$$

where  $\beta_{jk}^{mn}$  are complex numbers which can be determined by standard algorithms given the  $\tilde{A}_m$  operators and the  $\rho_j$  operators. Combining the last two expressions we have

$$\sum_{k} \sum_{mn} \chi_{mn} \beta_{jk}^{mn} \rho_k = \sum_{k} \lambda_{jk} \rho_k.$$
 (3.5)

From independence of the  $\rho_k$  it follows that for each k,

$$\sum_{mn} \beta_{jk}^{mn} \chi_{mn} = \lambda_{jk} \,. \tag{3.6}$$

This relation is a necessary and sufficient condition for the matrix  $\chi$  to give the correct quantum operation  $\mathcal{E}$ . One may think of  $\chi$  and  $\lambda$  as vectors, and  $\beta$  as a  $N^4 \times N^4$ matrix with columns indexed by mn, and rows by ij. To show how  $\chi$  may be obtained, let  $\kappa$  be the generalized inverse for the matrix  $\beta$ , satisfying the relation

$$\beta_{jk}^{mn} = \sum_{st,xy} \beta_{jk}^{st} \kappa_{st}^{xy} \beta_{xy}^{mn} . \tag{3.7}$$

Most computer algebra packages are capable of finding such generalized inverses. In appendix A it is shown that  $\chi$  defined by

$$\chi_{mn} = \sum_{jk} \kappa_{jk}^{mn} \lambda_{jk} \tag{3.8}$$

satisfies the relation (3.6). The proof is somewhat subtle, but it is not relevant to the application of the present algorithm.

Having determined  $\chi$  one immediately obtains the operator sum representation for  $\mathcal{E}$  in the following manner. Let the unitary matrix  $U^{\dagger}$  diagonalize  $\chi$ ,

$$\chi_{mn} = \sum_{xy} U_{mx} d_x \delta_{xy} U_{ny}^*. \tag{3.9}$$

From this it can easily be verified that

$$A_i = \sqrt{d_i} \sum_j U_{ij} \tilde{A}_j \tag{3.10}$$

gives an operator-sum representation for the quantum operation  $\mathcal{E}$ . Our algorithm may thus be summarized as follows:  $\lambda$  is experimentally measured, and given  $\beta$ , determined by a choice of  $\tilde{A}$ , we find the desired parameters  $\chi$  which completely describe  $\mathcal{E}$ .

#### IV. ONE AND TWO QUBITS

The above general method may be illustrated by the specific case of a black box operation on a single quantum bit (qubit). A convenient choice for the fixed operators  $\tilde{A}_i$  is

$$\tilde{A}_0 = I \tag{4.1}$$

$$\tilde{A}_1 = \sigma_x \tag{4.2}$$

$$\tilde{A}_2 = -i\sigma_y \tag{4.3}$$

$$\tilde{A}_3 = \sigma_z \,, \tag{4.4}$$

where the  $\sigma_i$  are the Pauli matrices. There are 12 parameters, specified by  $\chi$ , which determine an arbitrary single qubit black box operation  $\mathcal{E}$ ; three of these describe arbitrary unitary transforms  $\exp(i\sum_k r_k\sigma_k)$  on the qubit, and nine parameters describe possible correlations established with the environment E via  $\exp(i\sum_{jk}\gamma_{jk}\sigma_j\otimes\sigma_k^E)$ . Two combinations of the nine parameters describe physical processes analogous to the  $T_1$  and  $T_2$  spin-spin and spin-lattice relaxation rates familiar to us from classical magnetic spin systems. However, the dephasing and energy loss rates determined by  $\chi$  do not simply describe ensemble behavior; rather,  $\chi$  describes the dynamics of a single quantum system. Thus, the decoherence of a single

qubit must be described by more than just two parameters. Twelve are needed in general.

These 12 parameters may be measured using four sets of experiments. As a specific example, suppose the input states  $|0\rangle$ ,  $|1\rangle$ ,  $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$  and  $|-\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$  are prepared, and the four matrices

$$\rho_1' = \mathcal{E}(|0\rangle\langle 0|) \tag{4.5}$$

$$\rho_4' = \mathcal{E}(|1\rangle\langle 1|) \tag{4.6}$$

$$\rho_2' = \mathcal{E}(|+\rangle\langle +|) - i\mathcal{E}(|-\rangle\langle -|) - (1-i)(\rho_1' + \rho_4')/2 \quad (4.7)$$

$$\rho_3' = \mathcal{E}(|+\rangle\langle +|) + i\mathcal{E}(|-\rangle\langle -|) - (1+i)(\rho_1' + \rho_4')/2 \quad (4.8)$$

are determined using state tomography. These correspond to  $\rho'_i = \mathcal{E}(\rho_j)$ , where

$$\rho_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \tag{4.9}$$

 $\rho_2 = \rho_1 \sigma_x, \ \rho_3 = \sigma_x \rho_2, \ \text{and} \ \rho_4 = \sigma_x \rho_1 \sigma_x.$  From Eq.(3.4) and Eqs.(4.1-4.4) we may determine  $\beta$ , and similarly  $\rho_j'$  determines  $\lambda$ . However, due to the particular choice of basis, and the Pauli matrix representation of  $\tilde{A}_i$ , we may express the  $\beta$  matrix as the Kronecker product  $\beta = \Lambda \otimes \Lambda$ , where

$$\Lambda = \frac{1}{2} \begin{bmatrix} I & \sigma_x \\ \sigma_x & -I \end{bmatrix} , \tag{4.10}$$

so that  $\chi$  may be expressed conveniently as

$$\chi = \Lambda \begin{bmatrix} \rho_1' & \rho_2' \\ \rho_3' & \rho_4' \end{bmatrix} \Lambda, \tag{4.11}$$

in terms of block matrices.

Likewise, it turns out that the parameters  $\chi_2$  describing the black box operations on two qubits can be expressed as

$$\chi_2 = \Lambda_2 \overline{\rho}' \Lambda_2 \,, \tag{4.12}$$

where  $\Lambda_2 = \Lambda \otimes \Lambda$ , and  $\overline{\rho}'$  is a matrix of sixteen measured density matrices,

$$\overline{\rho}' = P^T \begin{bmatrix} \rho'_{11} & \rho'_{12} & \rho'_{13} & \rho'_{14} \\ \rho'_{21} & \rho'_{22} & \rho'_{23} & \rho'_{24} \\ \rho'_{31} & \rho'_{32} & \rho'_{33} & \rho'_{34} \\ \rho'_{41} & \rho'_{42} & \rho'_{43} & \rho'_{44} \end{bmatrix} P,$$
(4.13)

where  $\rho'_{nm} = \mathcal{E}(\rho_{nm})$ ,  $\rho_{nm} = T_n|00\rangle\langle00|T_m$ ,  $T_1 = I \otimes I$ ,  $T_2 = I \otimes \sigma_x$ ,  $T_3 = \sigma_x \otimes I$ ,  $T_4 = \sigma_x \otimes \sigma_x$ , and  $P = I \otimes [(\rho_{00} + \rho_{12} + \rho_{21} + \rho_{33}) \otimes I]$  is a permutation matrix. Similar results hold for k > 2 qubits. Note that in general, a quantum black box acting on k qubits is described by  $16^k - 4^k$  independent parameters.

There is a particularly elegant geometric view of quantum operations for a single qubit. This is based on the Bloch vector,  $\vec{\lambda}$ , which is defined by

$$\rho = \frac{I + \vec{\lambda} \cdot \vec{\sigma}}{2},\tag{4.14}$$

satisfying  $|\vec{\lambda}| \leq 1$ . The map Eq.(2.4) is equivalent to a map of the form

$$\vec{\lambda} \stackrel{\mathcal{E}}{\to} \vec{\lambda}' = M\vec{\lambda} + \vec{c}, \tag{4.15}$$

where M is a  $3\times3$  matrix, and  $\vec{c}$  is a constant vector. This is an *affine map*, mapping the Bloch sphere into itself. If the  $A_i$  operators are written in the form

$$A_i = \alpha_i I + \sum_{k=1}^3 a_{ik} \sigma_k, \tag{4.16}$$

then it is not difficult to check that

$$M_{jk} = \sum_{l} \begin{bmatrix} a_{lj} a_{lk}^* + a_{lj}^* a_{lk} + \\ \left( |\alpha_{l}|^2 - \sum_{p} a_{lp} a_{lp}^* \right) \delta_{jk} + \\ i \sum_{p} \epsilon_{jkp} (\alpha_{l} a_{lp}^* - \alpha_{l}^* a_{lp}) \end{bmatrix}$$
(4.17)

$$c_k = 2i \sum_{l} \sum_{ip} \epsilon_{jpk} a_{lj} a_{lp}^*, \qquad (4.18)$$

where we have made use of Eq.(2.3) to simplify the expression for  $\vec{c}$ .

The meaning of the affine map Eq.(4.15) is made clearer by considering the polar decomposition [15] of the matrix M. Any real matrix M can always be written in the form

$$M = OS, (4.19)$$

where O is a real orthogonal matrix with determinant 1, representing a proper rotation, and S is a real symmetric matrix. Viewed this way, the map Eq.(4.15) is just a deformation of the Bloch sphere along principal axes determined by S, followed by a proper rotation due to O, followed by a displacement due to  $\vec{c}$ . Various well-known decoherence measures can be identified from M and  $\vec{c}$ ; for example,  $T_1$  and  $T_2$  are related to the magnitude of  $\vec{c}$  and the norm of M. Other measures are described in the following section.

#### V. RELATED QUANTITIES

We have described how to determine an unknown quantum operation  $\mathcal{E}$  by systematically exploring the response to a complete set of states in the system's Hilbert space. Once the operators  $A_i$  have been determined, many other interesting quantities can be evaluated. A quantity of particular importance is the entanglement fidelity [8,16]. This quantity can be used to measure how closely the dynamics of the quantum system under consideration approximates that of some ideal quantum system.

Suppose the target quantum operation is a unitary quantum operation,  $\mathcal{U}(\rho) = U\rho U^{\dagger}$ , and the actual quantum operation implemented experimentally is  $\mathcal{E}$ . The entanglement fidelity can be defined as [16]

$$F_e(\rho, \mathcal{U}, \mathcal{E}) \equiv \sum_i \left| \operatorname{tr}(U^{\dagger} A_i \rho) \right|^2$$
 (5.1)

$$= \sum_{mn} \chi_{mn} \operatorname{tr}(U^{\dagger} \tilde{A}_{m} \rho) \operatorname{tr}(\rho \tilde{A}_{n}^{\dagger} U). \qquad (5.2)$$

The second expression follows from the first by using Eq.(3.1), and shows that errors in the experimental determination of  $\mathcal{E}$  (resulting from errors in preparation and measurement) propagate linearly to errors in the estimation of entanglement fidelity. The minimum value of  $F_e$  over all possible states  $\rho$  is a single parameter which describes how well the experimental system implements the desired quantum logic gate.

One may also be interested in the minimum *fidelity* of the gate operation. This is given by the expression,

$$F \equiv \min_{|\psi\rangle} \langle \psi | U^{\dagger} \mathcal{E}(|\psi\rangle \langle \psi|) U | \psi\rangle, \tag{5.3}$$

where the minimum is over all pure states,  $|\psi\rangle$ . As for the entanglement fidelity, we may show that this quantity can be determined robustly, because of its linear dependence on the experimental errors.

Another quantity of interest is the quantum channel capacity, defined by Lloyd [17,18] as a measure of the amount of quantum information that can be sent using a quantum communication channel, such as an optical fiber. In terms of the parameters discussed in this paper,

$$C(\mathcal{E}) \equiv \max_{\rho} S(\mathcal{E}(\rho)) - S_e(\rho, \mathcal{E}), \qquad (5.4)$$

where  $S(\mathcal{E}(\rho))$  is the von Neumann entropy of the density operator  $\mathcal{E}(\rho)$ ,  $S_e(\rho, \mathcal{E})$  is the entropy exchange [8], and the maximization is over all density operators  $\rho$  which may be used as input to the channel. It is a measure of the amount of quantum information that can be sent reliably using a quantum communications channel which is described by a quantum operation  $\mathcal{E}$ .

One final observation is that our procedure can in principle be used to determine the form of the Lindblad operator,  $\mathcal{L}$ , used in Markovian master equations of the form

$$\dot{\rho} = \mathcal{L}(\rho),\tag{5.5}$$

where for convenience time is measured in dimensionless units, to make  $\mathcal L$  dimensionless. This result follows from the fact that Lindblad operators  $\mathcal L$  are just the logarithms of quantum operations; that is,  $\exp(\mathcal L)$  is a quantum operation for any Lindblad operator,  $\mathcal L$ , and  $\log \mathcal E$  is a Lindblad operator for any quantum operation  $\mathcal E$ . This observation may be used in the future to experimentally determine the form of the Lindblad operator for systems, but will not be explored further here.

#### VI. QUANTUM MEASUREMENTS

Quantum operations can also be used to describe measurements. For each measurement outcome, i, there is associated a quantum operation,  $\mathcal{E}_i$ . The corresponding state change is given by

$$\rho \to \frac{\mathcal{E}_i(\rho)}{\operatorname{tr}(\mathcal{E}_i(\rho))},$$
(6.1)

where the probability of the measurement outcome occurring is  $p_i = \operatorname{tr}(\mathcal{E}_i(\rho))$ . Note that this mapping may be nonlinear, because of this renormalization factor.

Despite the possible nonlinearity, the procedure we have described may be adapted to evaluate the quantum operations describing a measurement. To determine  $\mathcal{E}_i$  we proceed exactly as before, except now we must perform the measurement a large enough number of times that the probability  $p_i$  can be reliably estimated, for example by using the frequency of occurrence of outcome i. Next,  $\rho'_i$  is determined using tomography, allowing us to obtain

$$\mathcal{E}_i(\rho_j) = \operatorname{tr}(\mathcal{E}_i(\rho_j))\rho_j', \tag{6.2}$$

for each input  $\rho_i$  which we prepare, since each term on the right hand side is known. Now we proceed exactly as before to evaluate the quantum operation  $\mathcal{E}_i$ . This procedure may be useful, for example, in evaluating the effectiveness of a quantum-nondemolition (QND) measurement [19].

### VII. CONCLUSION

In this paper we have shown how the dynamics of a quantum system may be experimentally determined using a systematic procedure. This elementary system identification step [20] opens the way for robust experimental determination of a wide variety of interesting quantities. Amongst those that may be of particular interest are the quantum channel capacity, the fidelity, and the entanglement fidelity. We expect these results to be of great use in the experimental study of quantum computation, quantum error correction, quantum cryptography, quantum coding and quantum teleportation.

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# APPENDIX A: PROOF OF THE $\chi$ RELATION

The difficulty in verifying that  $\chi$  defined by (3.8) satisfies (3.6) is that in general  $\chi$  is not uniquely determined by the last set of equations. For convenience we will rewrite these equations in matrix form as

$$\beta \vec{\chi} = \vec{\lambda} \tag{A1}$$

$$\vec{\chi} \equiv \kappa \vec{\lambda} \,. \tag{A2}$$

From the construction that led to equation (3.2) we know there exists at least one solution to equation (A1), which we shall call  $\vec{\chi}'$ . Thus  $\vec{\lambda} = \beta \vec{\chi}'$ . The generalized inverse satisfies  $\beta \kappa \beta = \beta$ . Premultiplying the definition of  $\vec{\chi}$  by  $\beta$  gives

$$\beta \vec{\chi} = \beta \kappa \vec{\lambda} \tag{A3}$$

$$= \beta \kappa \beta \vec{\chi}'$$
 (A4)  
$$= \beta \vec{\chi}'$$
 (A5)  
$$= \lambda .$$
 (A6)

$$= \beta \vec{\chi}' \tag{A5}$$

$$=\lambda$$
. (A6)

Thus  $\chi$  defined by (A2) satisfies the equation (A1), as was required to show.

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